Approximate Inference in Graphical Models using LP Relaxations

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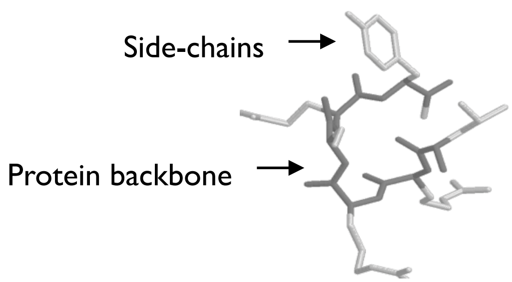
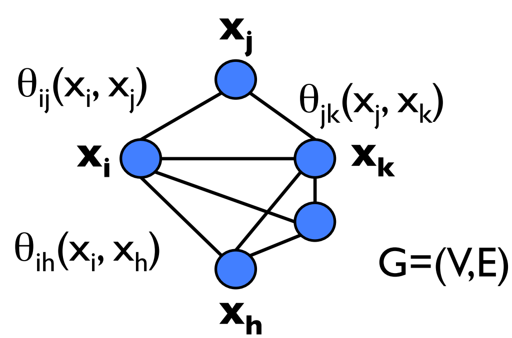
MAP in Undirected Graphical Models

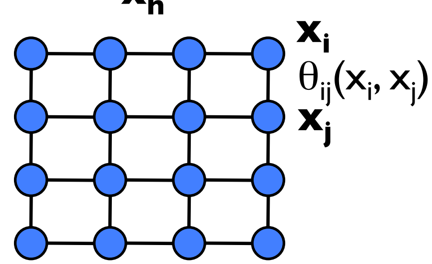
Real-world problems:



Protein design



Stereo vision



$$\Pr(x;\theta) \propto \exp\left(\sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \right)$$

Find most likely assignment:

$$x_{\text{map}} = \arg\max_x \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j)$$

How to solve MAP?

- MAP is known to be NP-hard (e.g., MAP on binary MRFs is equivalent to Max-Cut)
- Real-world MAP problems are not necessarily as hard as theoretical worst case

How to solve MAP?

- New toolkit: Message-passing algorithms based on linear programming relaxations

  (Schlensinger ’76, Kolmogorov & Wainwright ‘05, Vontobel & Koetter ‘06, Johnson et al. ’07, Komodakis et al. ‘07, Globerson & Jaakkola ’08…)

- Solves exactly when LP relaxation is tight: trees, binary submodular MRFs, and matchings
- In practice, we seldom have these structures
- By tightening the relaxation (problem specific), we *can* solve hard real-world problems, exactly

MAP as a linear program

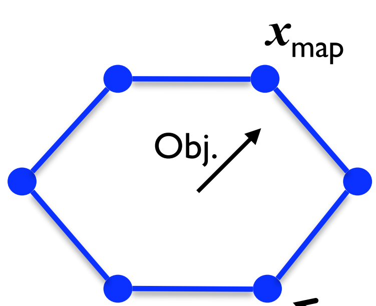
We can formulate the MAP problem as a linear program

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \boldsymbol{\theta_{ij}}(x_i, x_j) = \max_{\boldsymbol{\mu}\in\mathcal{M}(G)} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\,\theta_{ij}(x_i, x_j)$$

where the variables μ_{ij} are defined over edges.

The *marginal polytope* constrains the μ_{ij} to be marginals of *some* distribution:

$$\mathcal{M}(G) = \{\boldsymbol{\mu} \mid \exists \Pr(\boldsymbol{x};\boldsymbol{\theta}) \text{ s.t. } \mu_{ij}(x_i, x_j) = \Pr(x_i, x_j; \boldsymbol{\theta})\}$$

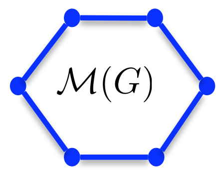


Very many constraints!

Vertices correspond to assignments

Relaxing the MAP LP

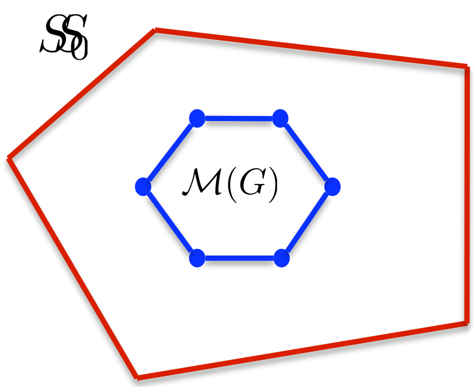
$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad = \quad \max_{\boldsymbol{\mu}\in\mathcal{M}(G)} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

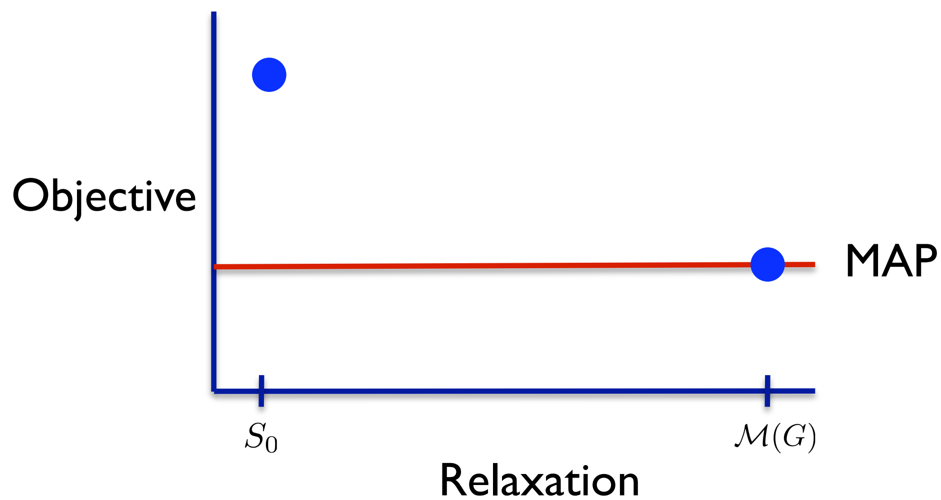


Relaxing the MAP LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

Such that $\mathcal{M}(G) \subseteq S$



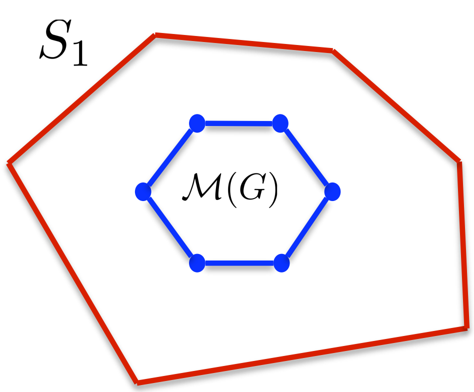


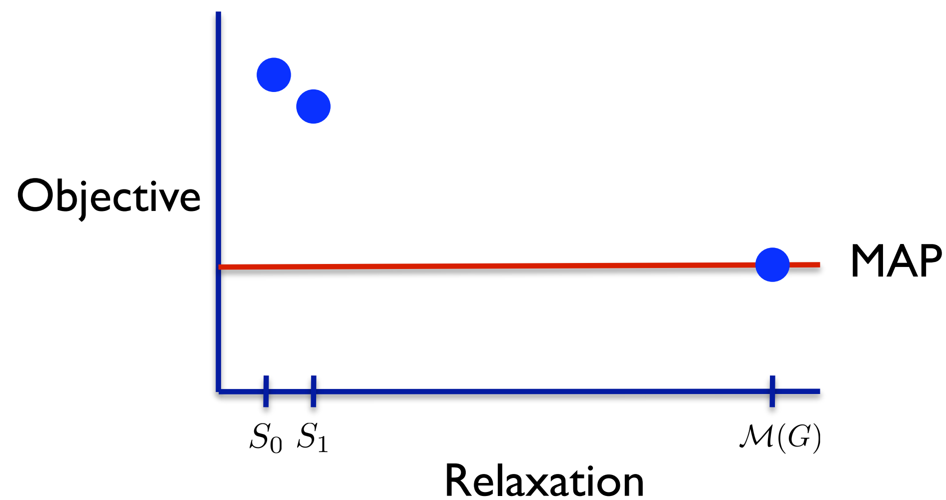
Simplest outer bound: $\sum_{x_i, x_j} \mu_{ij}(x_i, x_j) = 1$

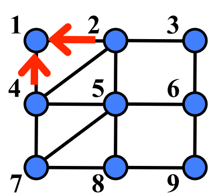
Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

Such that $\mathcal{M}(G) \subseteq S$







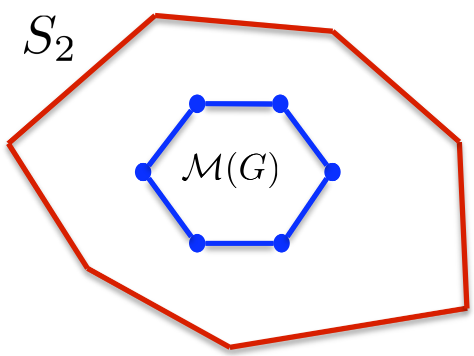
$$\sum_{x_2} \mu_{12}(x_1, x_2) = \sum_{x_4} \mu_{14}(x_1, x_4)$$

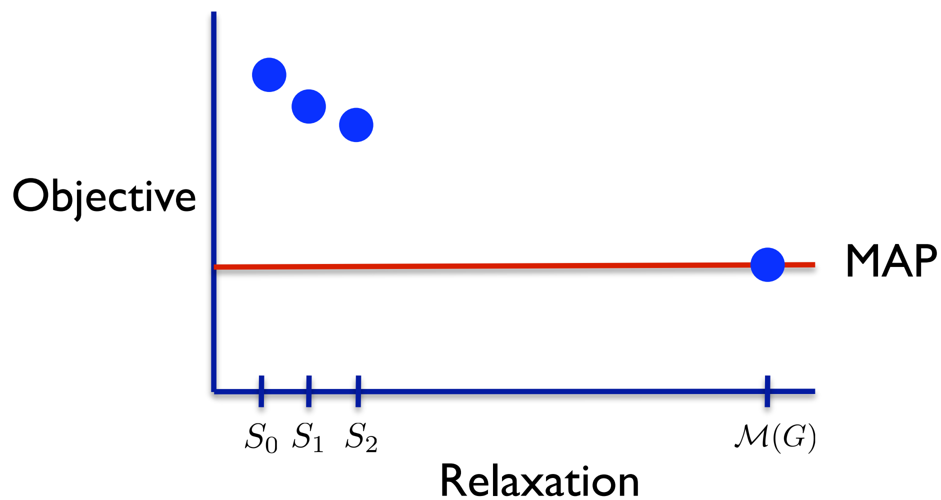
Partial pairwise consistency

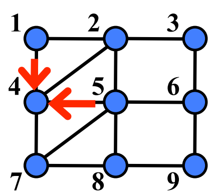
Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

Such that $\mathcal{M}(G) \subseteq S$





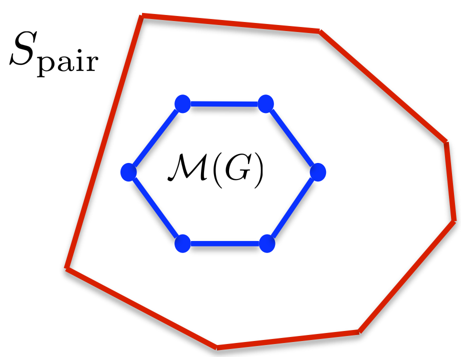


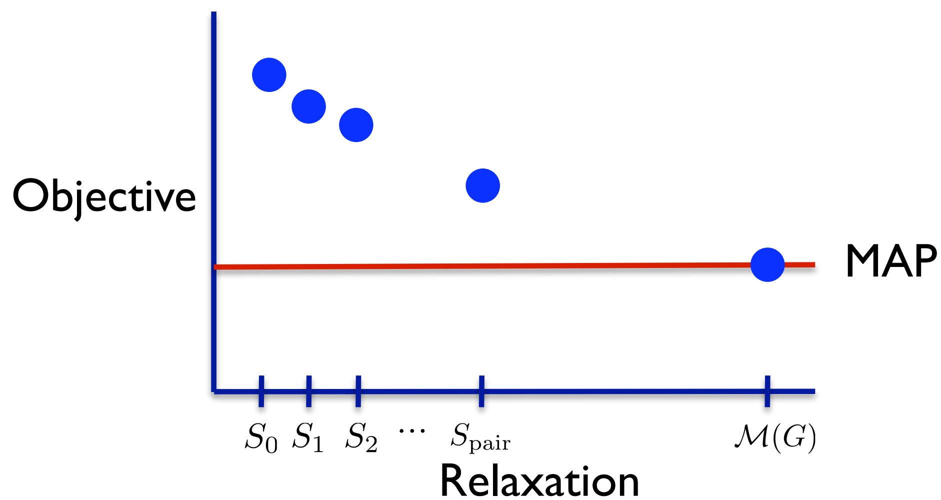
$$\left.\sum_{x_1} \mu_{14}(x_1, x_4) = \sum_{x_5} \mu_{45}(x_4, x_5)\right\} \quad \textit{Partial pairwise} \text{ consistency}$$

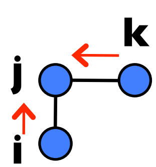
Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

Such that $\mathcal{M}(G) \subseteq S$







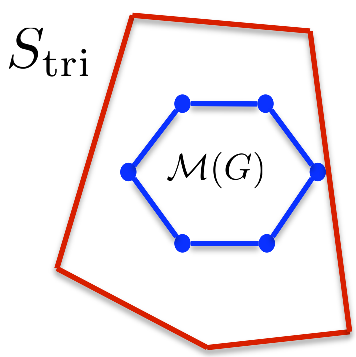
$$\left.\sum_{x_i} \mu_{ij}(x_i, x_j) = \sum_{x_k} \mu_{ij}(x_j, x_k)\right\}$$

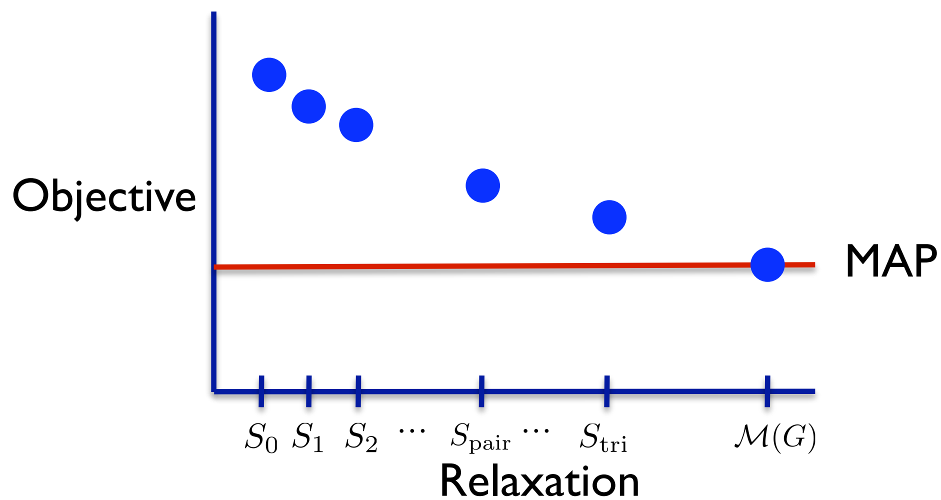
Pairwise consistency

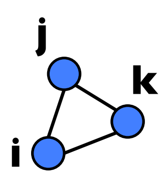
Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i, x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

Such that $\mathcal{M}(G) \subseteq S$







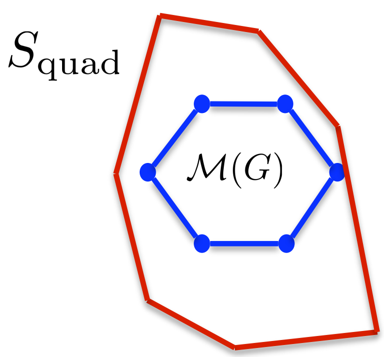
$$\boxed{\sum_{x_k} \mu_{ijk}(x_i, x_j, x_k) = \mu_{ij}(x_i, x_j)}$$

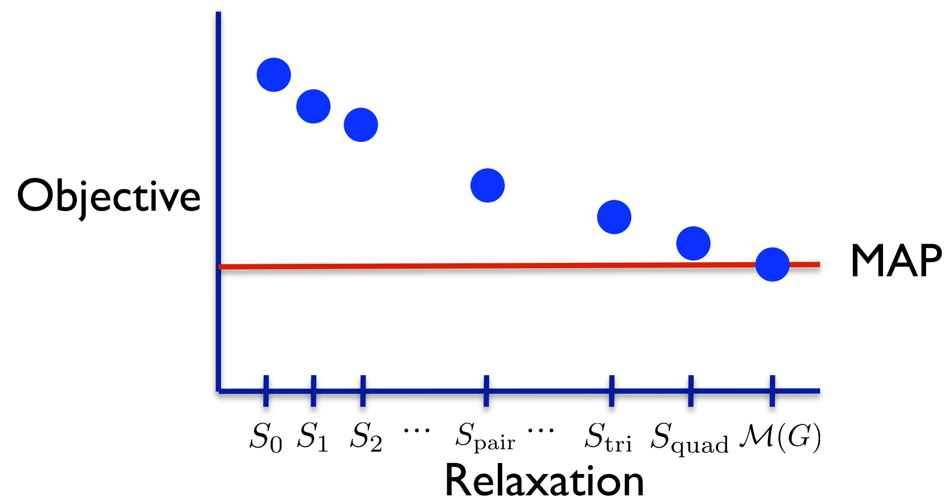
Triplet consistency

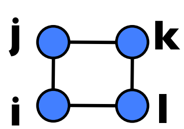
Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \leq \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i,x_j} \mu_{ij}(x_i,x_j)\theta_{ij}(x_i,x_j)$$

Such that $\mathcal{M}(G) \subseteq S$







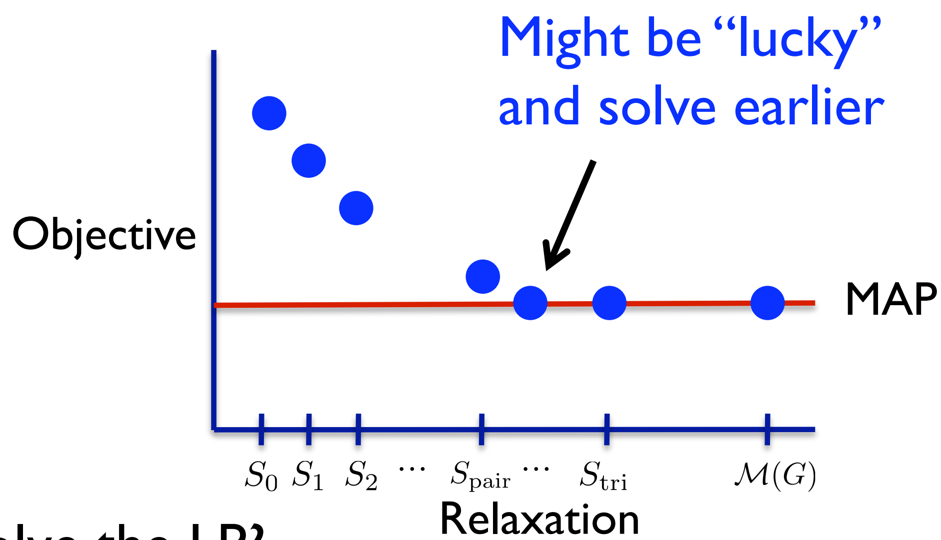
$$\boxed{\sum_{x_k,x_l} \mu_{ijkl}(x_i,x_j,x_k,x_l) = \mu_{ij}(x_i,x_j)}$$

Quadruplet consistency

Tightening the LP

$$\max_{\boldsymbol{x}} \sum_{(i,j)\in E} \theta_{ij}(x_i, x_j) \quad \le \quad \max_{\boldsymbol{\mu}\in S} \sum_{(i,j)\in E} \sum_{x_i,x_j} \mu_{ij}(x_i, x_j)\theta_{ij}(x_i, x_j)$$

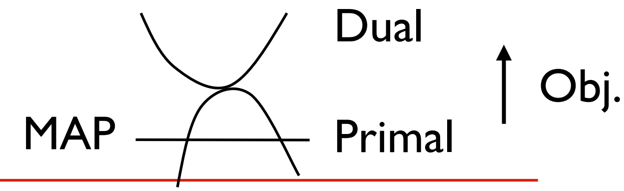
Such that $\mathcal{M}(G) \subseteq S$



Great! But…

- Can we efficiently solve the LP?
- What clusters to add?
- How do we avoid re-solving?

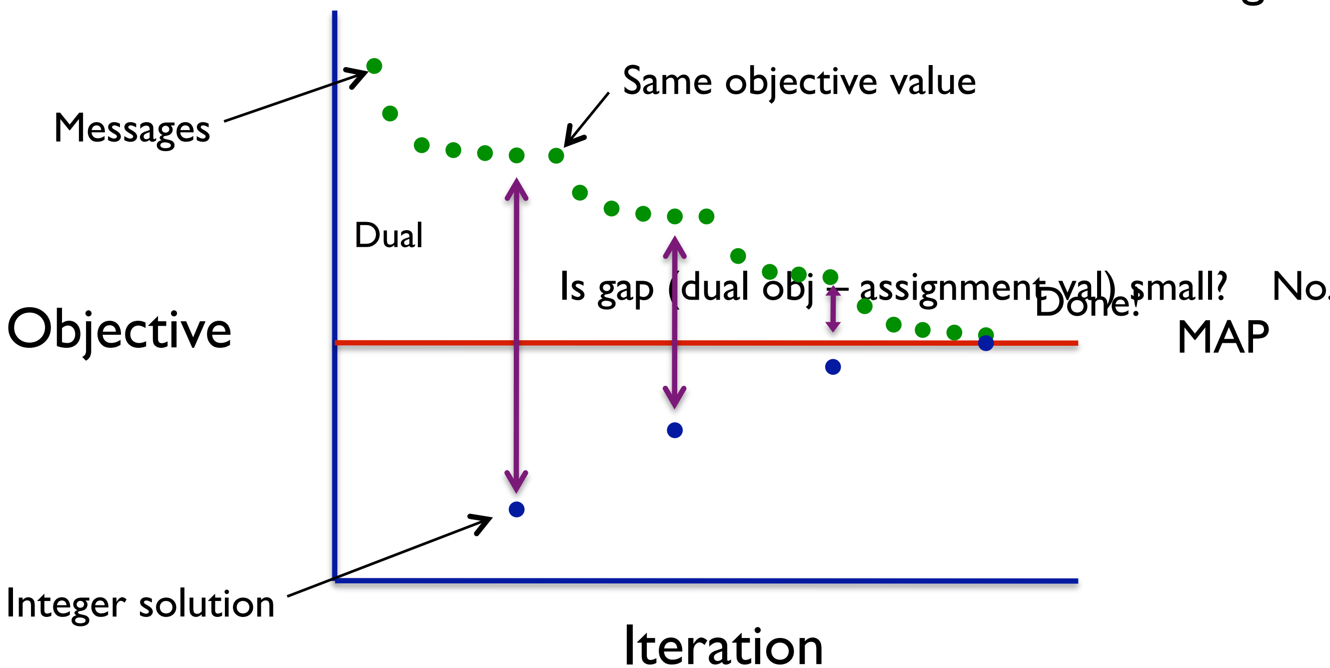
Our solution



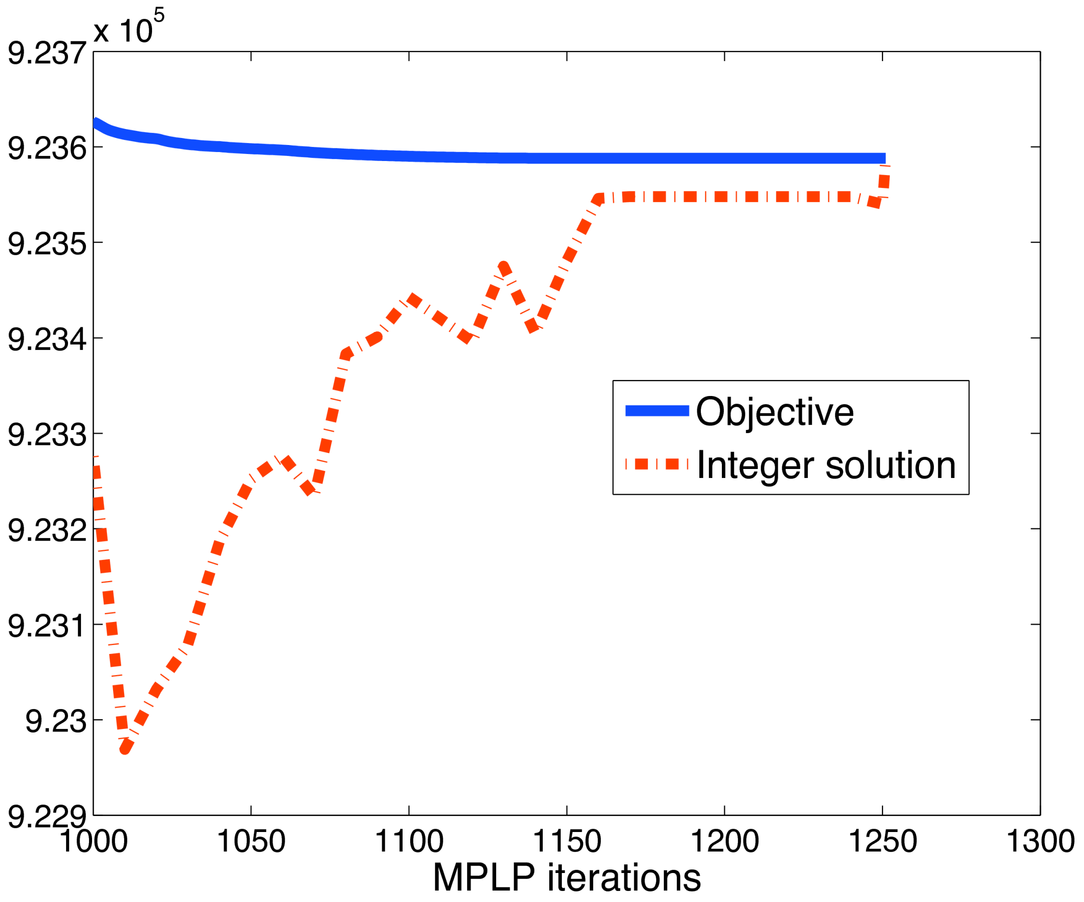
- Can we efficiently solve the LP?
  - We work in one of the *dual* LPs (Globerson & Jaakkola '07)
  - Dual can be solved by an efficient message-passing algorithm
  - Corresponds to coordinate-descent algorithm
- What cluster to add next?
  - We propose a greedy *bound minimization* algorithm
  - Add clusters with guaranteed improvement – upper bound gets tighter
- How do we avoid re-solving?
  - "Warm start" of new messages using the old messages

Dual algorithm

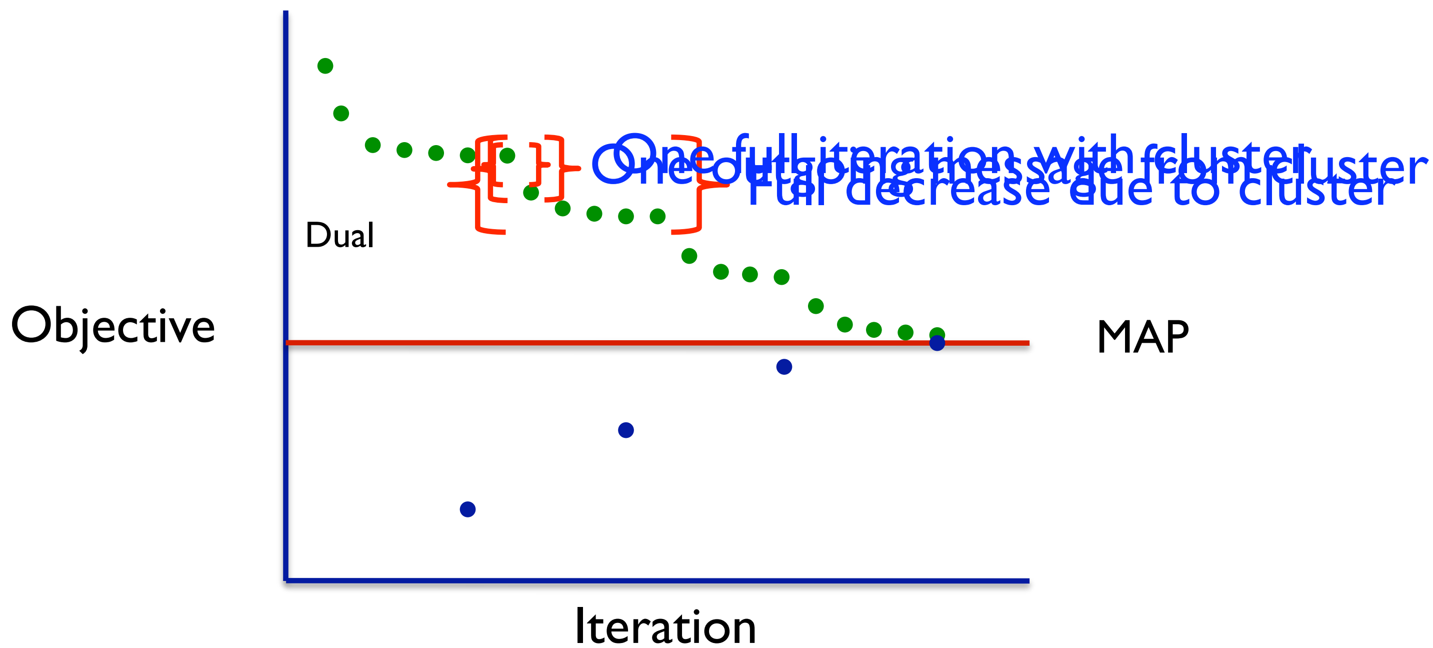
1. Run message-passing
2. Decode assignment from messages
3. Choose a cluster to add to relaxation
4. Warm start: initialize new cluster messages



Dual algorithm



What cluster to add next?



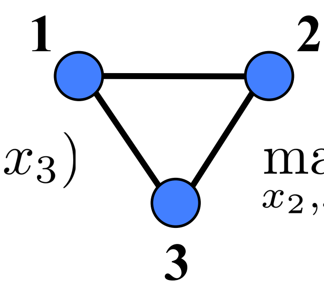
$$\sum_{e \in c} \max_{x_e} b_e(x_e) - \max_{x_c} \left[\sum_{e \in c} b_e(x_e) \right]$$

What cluster to add next?

$$\sum_{e \in c} \max_{x_e} b_e(x_e) - \max_{x_c} \left[\sum_{e \in c} b_e(x_e) \right]$$

$$\max_{x_1, x_2, x_3} \left[b_{12}(x_1, x_2) + b_{23}(x_2, x_3) + b_{13}(x_1, x_3) \right]$$

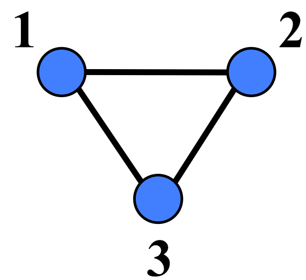
$$\max_{x_1, x_2} b_{12}(x_1, x_2)$$



$$\max_{x_1, x_3} b_{13}(x_1, x_3) \qquad \max_{x_2, x_3} b_{23}(x_2, x_3)$$

What cluster to add next?

$$\underbrace{\sum_{e \in c} \max_{x_e} b_e(x_e)}_{3*99} - \underbrace{\max_{x_c} \left[\sum_{e \in c} b_e(x_e) \right]}_{2*99-10}$$

$x_1 = 1$  $x_2 = 0$

$x_3 = 1$

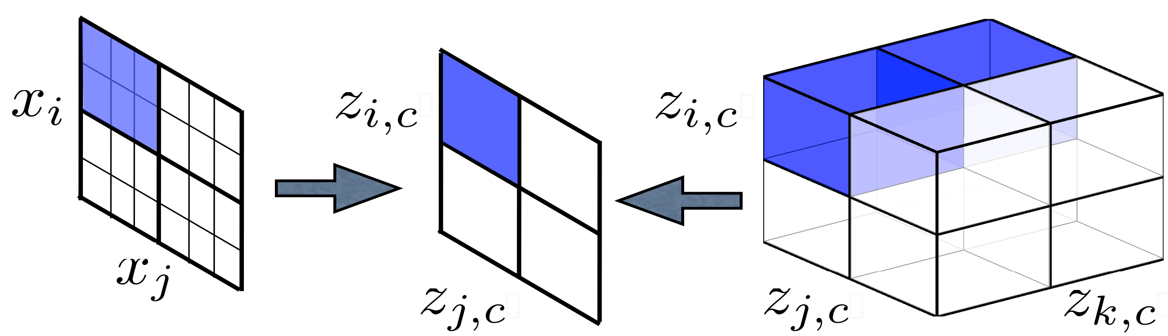
$b_{ij}(x_i, x_j) = 99$ if $x_i \neq x_j$

$b_{ij}(x_i, x_j) = -10$ otherwise

If dual decreases, there was frustration

Coarsened cluster consistency

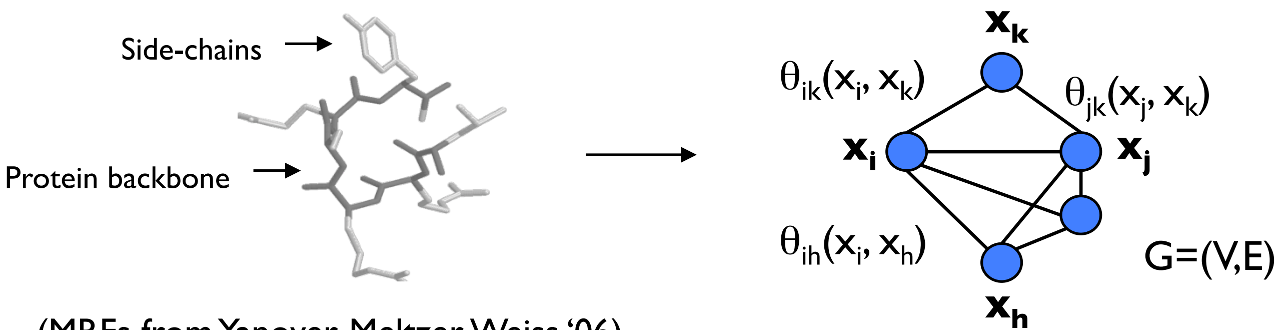
- Each new cluster requires adding a large number of LP variables $\mu_{ijk}(x_i, x_j, x_k)$ and constraints
- Is it possible to use just a subset of these constraints?
- We give a new class of *sparse* cluster constraints, enforcing consistency on *coarsened* variables



(Sontag, Globerson, Jaakkola, NIPS '08)

Experiments: Protein design

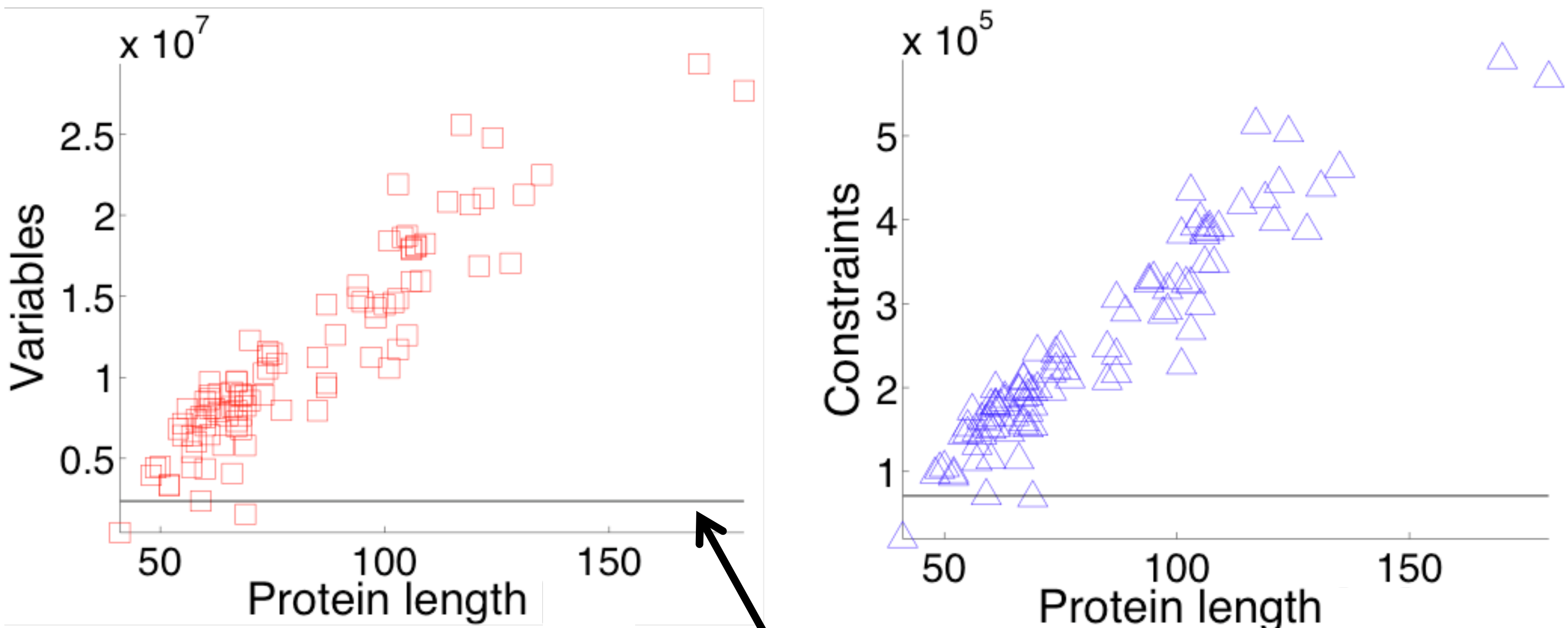
- Given protein's 3D shape, choose amino-acids giving the most stable structure



(MRFs from Yanover, Meltzer, Weiss '06)

- Each state corresponds to a choice of amino-acid and side-chain angle
- MRFs have 41-180 variables, each variable with 95-158 states
- Hard to solve
  - Very large treewidth
  - Many small cycles (20,000 triangles) and frustration

Primal LP, pairwise, is large



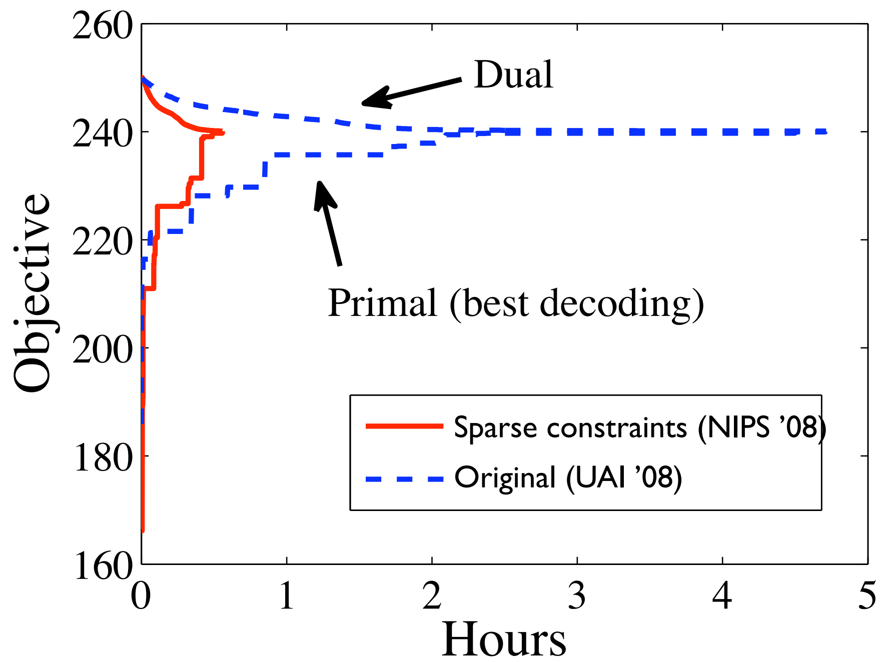
CPLEX can only run on 3:
must move to dual!

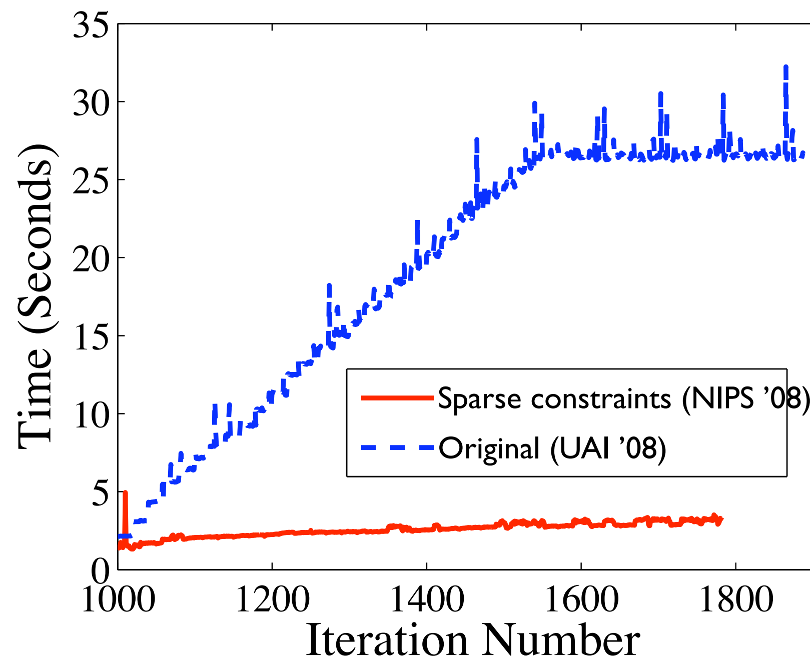
(Yanover, Meltzer, Weiss, JMLR '06)

Protein design results

- Pairwise constraints solve only 2 of the 97 proteins
- Iteratively tightening relaxation with triplets, we **exactly solve 96** of the 97 proteins (**!!!**)
- Using the coarsened clusters, average time to solve 15 largest proteins is 1.5 hours
- Bound criterion finds the right constraints: Only 5 to 735 triplets needed to be added per problem

Coarsening clusters really helps





Related Work

- Similar ideas can be done directly in the primal
  - Selection criteria of *constraint violation* instead of *bound minimization*
  - (Sontag & Jaakkola '08)

- Can also be applied to marginals
  - Guidance by bound on partition function rather than MAP value
  - Similar to region-pursuit algorithm for generalized BP (Welling UAI '04)

Conclusions & Future Work

- New toolkit of message-passing algorithms based on dual LP relaxations

  +

  Iterative tightening of LP relaxation

  =

  Ability to solve interesting real world-problems

- More generally, when can we expect these MAP inference techniques to be successful?

- How should we do learning with approximate inference – in particular, with LP relaxations?